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Modeling of the Interior Electric Field in Photovoltaic Cells

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ABSTRACT

With the emergence of photovoltaic technologies, there is a strong technological demand for high-performance photovoltaic devices. One of the most promising device concepts developed at SDSU is organic-based photovoltaic cells. The performance of the PV cells is controlled by charge generation and charge separation, and charge transportation processes. Extraordinary control over the properties of the organic photovoltaic materials will be needed in order for this research to succeed. Therefore, the interior electric field and the macro electric properties of the system are the foundation behind these facts and are critical properties on their performance. In this paper, the fundamentals of the interior electric field for these photovoltaic cells have been reviewed. Computer modeling by using finite element analysis combined with Monte Carlo method for these photovoltaic materials has been conducted for better understanding the performance of the cells. By creating multiple possible molecular distributions of a cell, many important issues such as the current flow and energy lost to the rising temperature have been compared.

Keywords: Photovoltaics, Solar Cell, Electric field, Modeling

INTRODUCTION

In today's society the solar cell could provide a much needed alternative to produce and sustain the quality of life that we live in today. The greatest advantage to using electricity created by photovoltaic cells is that it uses a resource that is never ending unlike the use of fossil fuels. The PV cell uses the suns energy to produce energy that does not harm the environment or add to global warming [1]. According to the US Department of Energy, "the amount of the sun's energy that reaches the Earth's surface every hour is greater than the total amount of energy that the world's human population uses in a year [2]." By researching and improving PV cells we could greatly reduce the negative effects impacting and destroying our environment daily.

Unlike previous uses of the sun's light, such as solar panels to create heat, photovoltaic cells can actually store energy in a battery and use it later as electricity [3]. This process is known as the photoelectric effect. A photovoltaic cell creates electricity by first absorbing the sun's rays. These rays are made up of photons. Photons are small individual particles that carry an amount of energy. The amount of energy that is carried by each photon is determined by its wavelength. This energy and the band gap energy of the PV cell determine which wavelengths can be used to create electricity.

The band gap energy of a material is the difference between the valence band and the conduction band. These are the lowest and highest energy levels for an electron, also known as when the electron is in a bound state or a free state. It is this difference that determines what photons are too weak to free an electron which in turn pass through or are reflected away from the PV cell. Some examples of different materials band gap energies are shown in Figure 1. The energy that is absorbed is transferred into the electrons within the atoms in the PV cell. It is at this time, due to the extra energy gained by each electron, they are able to escape their bound state in the semiconductor material that makes up the PV cell and roam freely and in turn become a part of the electrical current in the cell.

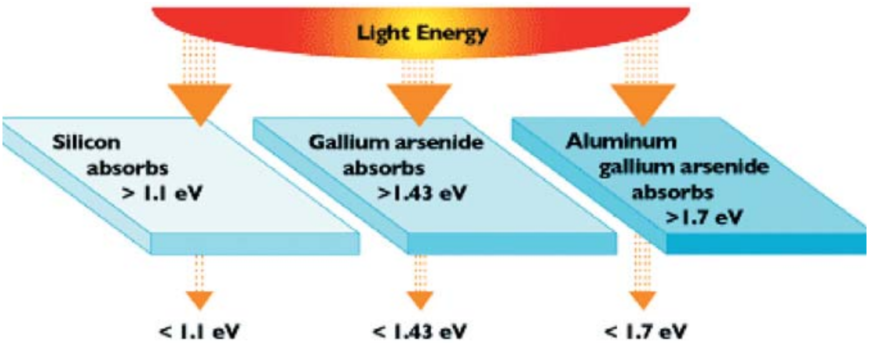

Figure 1. Band gap energies for silicon, gallium arsenide, and aluminum gallium arsenide.

Another aspect of the makeup of the PV cell includes an “n” layer and a “p” layer, see Figure 2. These layers are made up of extra electrons and holes respectively. The way these two layers are put together form a junction which in turn creates an electric field [2]. The semiconductor material and this junction together cause an electrical current to freely run through the PV cell. This current is then able to pick up the electrons that escape the semiconductor material and bring them to the external load, shown in Figure 3.

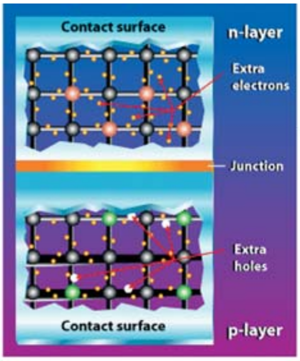

Figure 2. P and N type layers, extra holes and electrons.

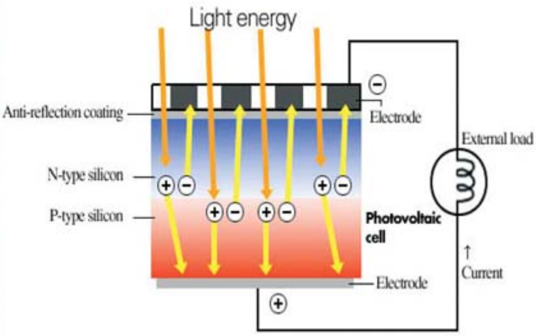

Figure 3. Current to external load.

Currently the use of PV cells is minimal. The main reason for this is the cost. Although this is something that is being worked on, the fact that the efficiency of a PV module or array is still less than 25% greatly impacts people not to invest in them yet. However, the improvements being made on where the modules and arrays can be placed, such as roof tops and inside skylights, is very promising.

Some major aspects of a PV cell that affect its performance is the band gap energy that its material make up has, the amount of reflected light, as well as the elements resistance. Over two thirds of the energy lost from the sun light is due to the photons that do not have enough energy to remove an electron and the photons that have more than enough energy. The reason that the photons with more than enough energy cause energy loss as well is because the energy not used to remove an electron cannot be used elsewhere so it is simply discarded.

One way to improve a PV cell's efficiency would be to work on a way to lower the band gap energy but still have the highest power. As stated before, the power output of the PV cell is the current times the voltage. The voltage is also affected by the band gap energy because the lower the band gap energy the lower the voltage becomes. Overall, you must find the most efficient combination for the band gap energy to absorb the most photons to create the highest current while keeping the voltage as high as possible within the PV cell.

Another key part of a photovoltaic cell is the molecules that make it up. The two main phases that exist in a molecule are acceptor and donor, each with important traits. An electron donor helps the semiconductor in the cell by giving up one or more conduction electrons which is done by becoming ionized/positively charged [4]. Similar to the donor, the accepter also helps the semiconductor. However, the acceptor gains the given electrons in order to create holes in the conduction band [4]. The results of having both donor and acceptor are that of the conduction band, which allows current flow across the PV cell, in turn creating electricity. Shown in Figure 4 is the photovoltaic process which only occurs due to the electron donor and acceptor.

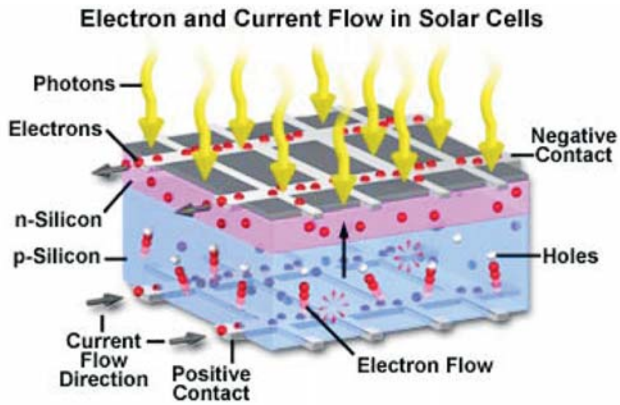

Figure 4. Photovoltaic process.

THEORY

This research strongly relies on the understanding of the electromagnetic field and use of three-dimensional finite element analysis based on Maxwell's equations governing classical electromagnetic propagation in dielectrics. Maxwell's equations provide the mathematical basis for rigorous analysis of classical electromagnetic wave propagation. Maxwell originally proposed an arcane system of 20 equations in 20 unknowns. The system was subsequently simplified by Heaviside and Hertz to its modern form, namely [5, 6]

$$-\dot{\boldsymbol{B}} = \nabla \times \boldsymbol{E}, \quad \dot{\boldsymbol{D}} + \boldsymbol{J} = \nabla \times \boldsymbol{H} \tag{1}$$

Where **B** is magnetic induction, **E** is electric field intensity, **D** is electric displacement, **J** is current density, and **H** is magnetic field intensity. Continuity of **E** and **H** is required in order to define the spatial derivatives. Note that in (1) bold letters represent vectors, $\nabla\times$ is the curl operator, and time derivatives are denoted by a dot above the variable.
The weak form of the scalar integral operator available to be applied in the conventional finite element formulation is

$$\int_{\Omega} G \cdot \left(\varepsilon \ddot{E} + \sigma \dot{E}\right) d\Omega \equiv -\frac{1}{\mu}\int_{\Omega} \nabla \times \boldsymbol{E} \cdot \nabla \times \boldsymbol{G} d\Omega - \frac{1}{\mu}\int_{\Sigma} \mathbf{G} \cdot \boldsymbol{n} \times \nabla \times \boldsymbol{E} d\Sigma \tag{2}$$

Where Ω is the domain of integration, Σ is its boundary, and n is the outward unit normal vector to Σ. Proportionality factors, μ, ε, and σ, are magnetic permeability, dielectric permittivity, and conductivity, respectively. G is the so-called test function over the wave domain.

Given the above mathematical preamble, the finite element procedure consists of partitioning or discretizing interior domain Ω into a number of subdomains or finite elements. The field is approximated over each element by an interpolating or shape function depending on values at discrete notes on or in the element. Consider a 3-dimensional 8-node element, as shown in Figure 5, having a 3-D magnetic, thermal, electric field capability with limited coupling between the fields. The shape function matrix and node vector for element m are written as

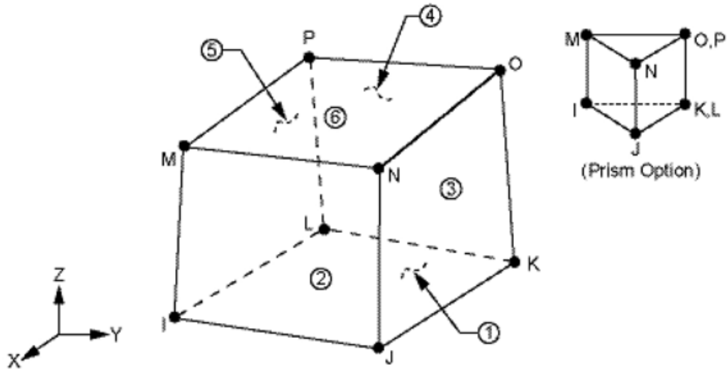

Figure 5. 3-D 8-node coupled-field element geometry.

$$\boldsymbol{S}^m(\boldsymbol{x}) \equiv \begin{bmatrix} S^m(x) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & S^m(x) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & S^m(x) \end{bmatrix}, \quad \boldsymbol{f}^m(\boldsymbol{t}) \equiv \begin{bmatrix} f_1^m \\ f_2^m \\ f_3^m \end{bmatrix} \tag{3}$$

Where $S^m(x)$ and 0 are row 8-vectors and $f_K{}^m(t)$ are column 8-vectors for the three field components.

All of the above information is already programmed into the ANSYS program that is used to find the desire data for this research.

In order to completely understand the process and results of this research, generating molecular distribution (donors and acceptors) in the given materials with desired volume percentage by using Monte Carlo Method, i.e., the random number function in the Microsoft Excel program, is also very important. The first step is to generate a random number. The function to do this is =rand(). This generates a number between 0 and1. However, the process does not end here because unless you want to go through my hand and determine if it is above or below the percentage cut off you must also understand the if function. The function you have to type in the cell this time is something similar to the following, =IF(B1>0.3333,1,2). The way this function works is you first specify the cell with the random number, B1. Next you use a greater than or less than sign, in my case it is greater than. Following that you must specify the percentage. In my case I used 33.33%, which is equivalent to 0.3333. Then after inserting a comma you must specify if the function is true what the number should change to. This means that if B1 is greater than 0.3333 then it changes to a 1. In the function a second comma is inserted to define what happens if the function is false. In this case, if B1 I less than 0.3333 then the cell changes the number to 2. With the understanding of this information you will now be able to understand the remainder of my research.

MODEL, RESULTS, AND DISCUSSION

Finite element analysis is a way to solve a problem with too many questions. The way it works is by making assumptions that simplify the problem to the point that it becomes solvable with the resources you have [4]. By dividing up the given cell area into many elements (pieces), we are able to become more accurate with our work and solution. In this work, a cube with dimension of 10 μm × 10 μm × 10 μm is chosen and split into 30 times in each direction. This in turn breaks the one cube into 27,000 tiny cubes.

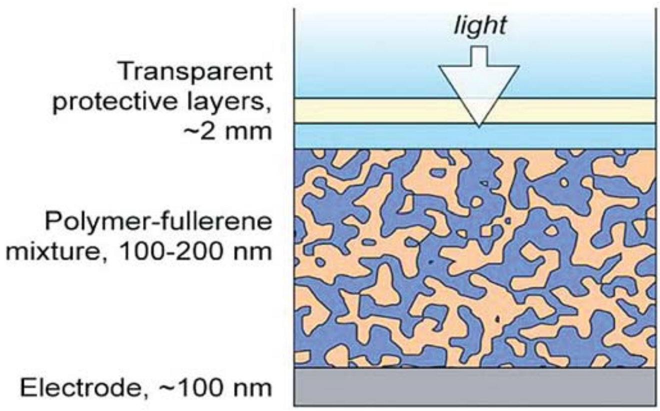

Figure 6. Example of a solar cell's distribution.

In order to continue solving the given problem you must know the makeup of each overall cell. This means that we must know the distribution of acceptor and donor phases. In order to do this we must first know what the percentage of each is, as shown in Figure 6 [7]. For one of my cells, the chosen breakdown for my first model was 1:1, meaning that 50% are donor and 50% are acceptor phases. I then used the Monte Carlo method to get a random distribution. In order to do this I used the random number function in excel. I used this function 27,000 times so that I would have one entry per small cell. Each of these numbers was a real number between 0 and 1. From there, I used the if function to change all of the numbers greater than or equal to 0.5 to 1 and all numbers less than 0.5 to equal 2. By doing this I was able to label ever one of the 27,000 tiny cells within my overall cell either an electron acceptor phase or an electron donor phase.

I repeated this process for my second model. For this model I used a 1:2 ratio. This in turn means that my model would have 33.333% of one phase and 66.666% of the other phase. Overall the same process was used for both models but with two different distributions sets.

Then I used my distribution and inserted it into the input batch file to run the program. This batch file included the size of the film with periodic boundary conditions, the size of the phases and the number of sub cells to be used, and the electric resistance constants as well as other constants. This file also discussed the starting temperatures of both sides of the solar cell and the thermal conductivity. With all of the correct figurations and wording, this file works to run in the desired program.

Next I ran the ANSYS program. With this program I was able to look at my results and compare my two different volume ratios of donor-acceptor phase distributions. I was also able to look at specific properties of the cell after the voltage had been applied. Along with a 3D model of what my distribution looks like, I looked at the electric distribution that occurs, the current flow of the electric field and lastly the temperature change over the time that the voltage is applied and after.

For my first model I used a 1:1 volume ratio of donor-acceptor phase. This means that my model has 50% donor and 50% acceptor phases. Shown in Figure 7 is the distribution of model 1 which was generated using the Monte Carlo Method. By use of Finite Element analysis I was able to generate a 3-D model of the electric field contour, see Figure 8. I was also able to generate a vector simulated 3-D model of the distribution of the electric field current flow, shown in Figure 9. Figure 10 shows the change in temperature for model 1 assuming it started at 17.5°C and change that occurred when the voltage was applied.

Similar to the first model, Figure 11 shows the distribution of the second model that has a 1:2 volume ratio of donor-acceptor phases. There are noticeably less purple squares in this distribution which represents 33.33% volume of the donor phase and the blue represents 66.67% volume of the acceptor phase. Figure 12 shows slightly more rigid contours for model 2 distribution of the electric field. The distribution of the electric field current flow for model 2 is shown in Figure 13. The temperature change for model 2 is shown in Figure 14, there is a similar curve to the graph for model 1 but the final temperature is around 20 degrees less.

Below are the images that I collected from the ANSYS program.

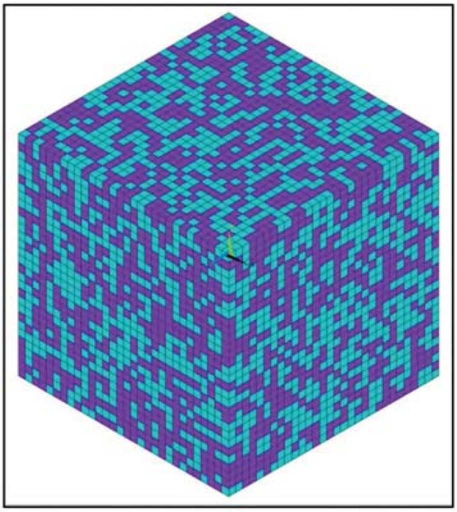

Figure 7. Distribution of donor (purple) and acceptor (blue) phases in model 1 (volume ratio 1:1).

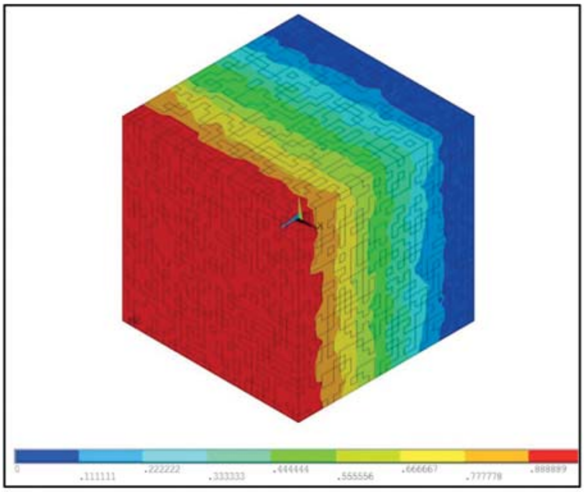

Figure 8. Electric potential distribution of model 1.

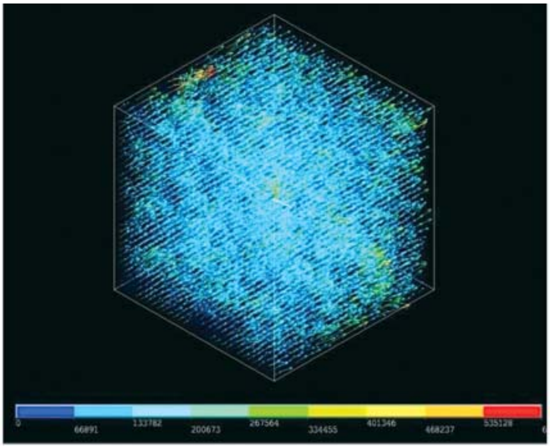

Figure 9. Electric field current flow of model 1.

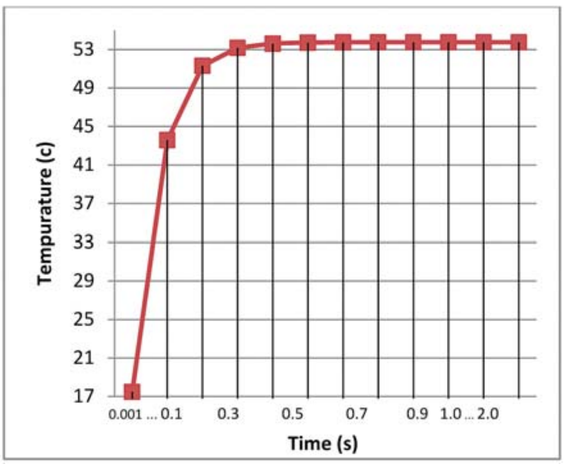

Figure 10. Change in temperature of model 1.

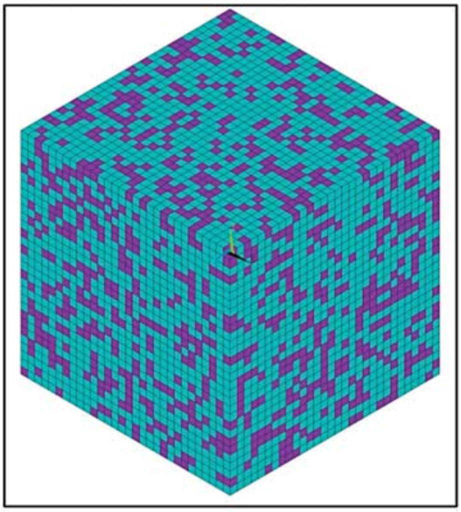

Figure 11. Distribution of donor (purple) and Acceptor (blue) phases in model 2 (volume ratio 1:2).

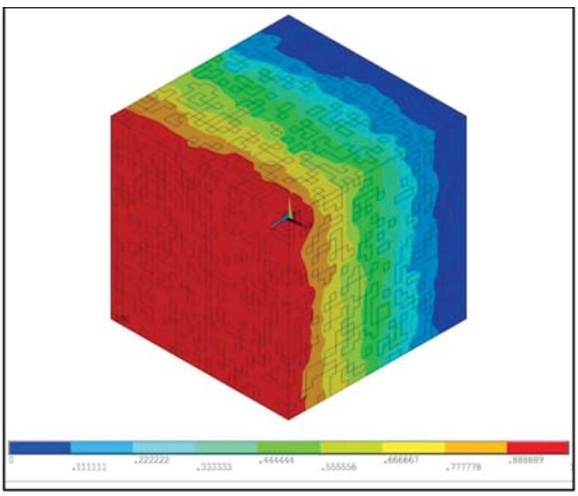

Figure 12. Electric potential distribution of model 2.

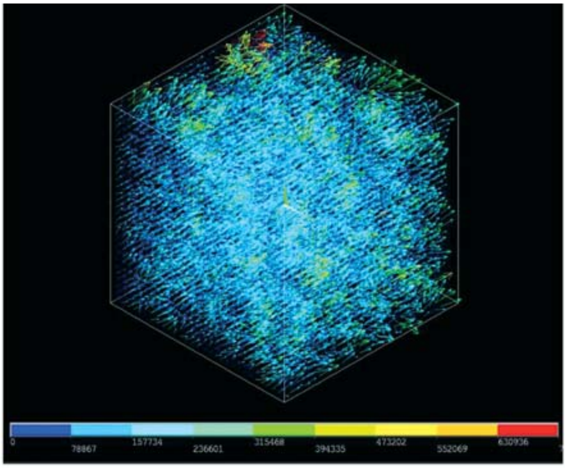

Figure 13. Electric field current flow of model 2.

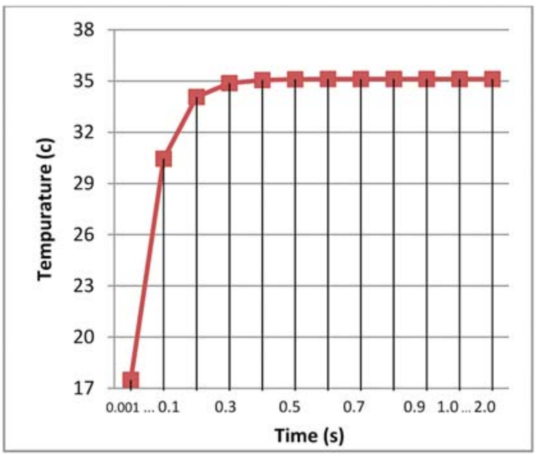

Figure 14. Change in temperature of model 2.

CONCLUSION

The research has shown us the capabilities that we have with this software to test and improve photovoltaics. The tests that I performed allowed us to compare first of all how the electric field is distributed. A benefit of this test is that we can see what distribution best allows for a current to flow throughout the cell. With this we would be able to better determine how the cell will create electricity from the sun light's photons. We are better able to determine the current flow by looking at the diagrams such as the ones I have included above. When you look at this image on a large enough scale you are able to see the arrows showing the way that the voltage flows through the cell.

Another important benefit to this ANSYS program is that it allows us to observe the distribution without having to plot it by hand. This is very beneficial because of its very minute scale and the amount that you subdivide it. Without this software you would spend an overwhelming amount of time on just the distribution.

The last aspect of the cell that I looked at was the change in the temperate due to the applied voltage and environment's temperature. By assumption we can look at the graphs and notice that both models started with a similar temperature, our specified 17.5 degrees, but jumped after the voltage was applied. From there, the temperature steadily rose until it maxed out and stayed at a constant temperature. The benefit this assumption gives us is that we will be able to compare what distribution creates the least heat. It would be logical to assume that with a lower temperature less electricity would be lost, therefore creating a more efficient cell.

Overall, my trials showed us the possibilities that the ANSYS program has regarding the interior electric field of a photovoltaic cell. With more data and specific information, there is continued hope for improvement for the photovoltaic cells. By running test similar to mine on more distributions, more trends will be discovered, and in turn more improvements can be found and applied.

ACKNOWLEDGEMENTS

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